DNA unzipping and the unbinding of directed polymers in a random media.

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(Dated: February 6, 2008)

We consider the unbinding of a directed polymer in a random media from a wall in $d = 1 + 1$ dimensions and a simple one-dimensional model for DNA unzipping. Using the replica trick we show that the restricted partition functions of these problems are *identical* up to an overall normalization factor. Our finding gives an example of a generalization of the stochastic matrix form decomposition to disordered systems; a method which effectively allows to reduce dimensionality of the problem. The equivalence between the two problems, for example, allows us to derive the probability distribution for finding the directed polymer a distance z from the wall. We discuss implications of these results for the related Kardar-Parisi-Zhang equation and the asymmetric exclusion process.

The problem of a directed polymer in a random media (DPRM) has received much attention for more than two decades [1]. This stems from many reasons: It is a relevant model for a single vortex in a disordered type-II superconductor [2] and it is one of the simplest examples of disordered systems for which, in some cases, exact result can be obtained. Moreover, the model maps both to the Kardar-Parisi-Zhang (KPZ) equation [3], which is perhaps the simplest non-linear stochastic growth equation, and to the noisy Burger's equation [4]. The latter, in one dimension, describes the long-time and large length-scale behavior of asymmetric exclusion processes (ASEP) [5, 6], which have been studied as prototypes of non-equilibrium systems [7, 8]. The relations between the different models has been extremely fruitful: in some cases results which are hard to derive in one model can be easily obtained using another.

Here we present a new, more subtle, relation between the DPRM problem and the DNA unzipping problem [9]. In particular, we consider (a) the depinning of a DPRM from an attractive wall in $d = 1 + 1$ dimensions and (b) the force induced unzipping of a directed elastic line (in $d \geq 1+1$ dimensions) from a disordered columnar defect. We study a low temperature limit where the only excursion of the line from the defect occurs at the edge of the sample where the external force is acting (see Fig. 1). Both problems are disordered. In the DPRM problem the half-plane is taken to have uncorrelated point disorder, while in the unzipping problem there is uncorrelated point disorder localized on the columnar defect. In the DPRM problem it is well known that as the strength of the disorder grows there is an unbinding transition whereby the polymer leaves the wall. Similarly, it is known that in the unzipping problem as the force acting on the line exceeds a critical value, the line leaves the potential. The unzipping model has been recently used in the context of single molecule experiments performed on DNA [9, 10, 11] and also in relation to magnetic force microscopy experiments in type-II superconductors [12].

Both problems have been treated in some detail before and superficially bear little resemblance. For example, the unbinding of the DPRM is a continuous phase transition while the unzipping problem is a first-order phase transition. More interesting, the dimensionality of the problems is different. As we show the unzipping problem is effectively one-dimensional, while the DPRM problem is two dimensional. Nevertheless, we find that below the unbinding/unzipping transitions the replicated partition function of the DNA unzipping model is *identical* to the replicated generating function for the localization length of the polymer near the wall. Such an identity allows us to apply all known results from the unzipping problem to the DPRM unbinding problem. For example, we can derive the distribution function of the DPRM localization length near the wall below the transition. This identity also allows one to perform large scale numerical simulations of the DPRM by effective reduction of the dimensionality of the problem.

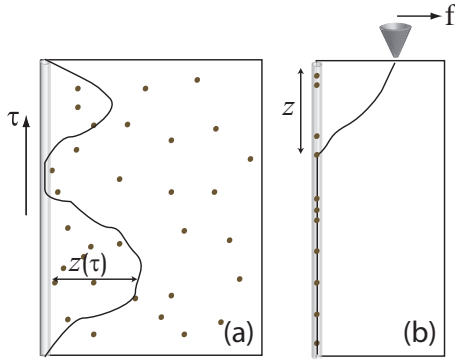

FIG. 1: The two problems discussed in the text. (a) Unbinding of a line from an attractive wall in the presence of point disorder in $d = 1 + 1$. (b) Unzipping of a line with point disorder confined to an attractive line.

We also discuss the implication of our result to both the KPZ equation and the ASEP. When the DPRM model is mapped to the KPZ equation, the wall acts as a free boundary condition for the growing interface and the attractive potential reduces the growth locally near the interface. The transition is approached by increasing the local growth rate at the interface. The relation to the unzipping problem allows us to derive the distribution function for the height profile near the transition. When

the DPRM is mapped to an ASEP the boundary corresponds to particles being injected at the end of a semi-infinite system with a rate which is slower than the particle hopping rate in the bulk of the system. Here the transition is approached by increasing the injection rate of particles. Using our results we discuss the structure of the particle density near the transition. The relation between the models suggests a deeper relation which may not be transparent in our derivation.

Equivalence between a two-dimensional (2d) unbinding problem and a one-dimensional (1d) unzipping problem is quite remarkable because lower dimensional problems are generally much easier to deal with. Without disorder our results can be understood in the context of stochastic matrix form (SMF) decomposition [13] as follows. First, we map the partition function of a 2d classical problem (DPRM) into the partition function of a quantum 1d problem, where the coordinate along the polymer is replaced by an imaginary time. Next we interpret the ground state wave-function of this quantum problem as a partition function of another classical 1d problem (DNA unzipping). The latter step is called SMF decomposition. Here we present an example extending this method to a disordered problem which corresponds to a Hamiltonian which depends on (imaginary) time. We believe that our findings can be further generalized to a wider class of disordered problems.

Unzipping of an elastic line from a columnar pin. Let us consider an external force $\mathbf{f}$ pulling the top end of a line from an attractive disordered columnar pin (see Fig. 1b). Neglecting excursions of the bound part of the line into the bulk, we can write the partition function as a sum over positions z where the line leaves the pin. The contribution of the unzipped part can be easily computed from the elastic energy [12]:

$$\mathcal{F}_0(z) = -\mathbf{f}\cdot\mathbf{r}(\mathbf{0}) + \int_0^z dz' \left[\frac{\gamma}{2}(\partial_{z'}\mathbf{r}(z'))^2\right]. \qquad (1)$$

Here $\mathbf{r}(z)$ denotes transverse coordinates of the line and z is the coordinate parallel to the defect. Integrating over all possible paths gives the corresponding free energy: $F_0(z) = -f^2 z/2\gamma$ [19]. The free energy of the bound part, up to a constant, is $F_1(z) = V_0(L-z) + \int_z^L dz' U(z')$, where V_0 is the value of the attractive potential, L is the length of the columnar defect which is assumed to be very large, and $U(z)$ is a random uncorrelated potential with zero mean satisfying $\overline{U(z_1)U(z_2)} = \Delta\delta(z_1 - z_2)$.

The partition function Z is a sum of the corresponding Boltzmann weights over all possible values of z [12]:

$$Z = \int_0^L Z(z) = \int_0^L dz\, \mathrm{e}^{-F_{\rm uz}(z)}, \qquad (2)$$

where up to an unimportant constant additive term $V_0 L$:

$$F_{\rm uz}(z) = F_0(z) + F_1(z) = \epsilon z + \int_z^L dz' U(z'). \qquad (3)$$

For simplicity we work in the units, where $k_B T = 1$. In the equation above $\epsilon = (f_c^2 - f^2)/2\gamma$, where f is the force applied to the end of the flux line and $f_c = \sqrt{2\gamma|V_0|}$ is the critical force. Note that the partition function (2) describes effectively a one-dimensional problem. The statistical properties of the unzipping transition can be obtained by replicating Eq. (2) [14]:

$$Z_n \equiv \overline{Z^n} = \overline{\int_0^L dz_1 \ldots \int_0^L dz_n\, \mathrm{e}^{-\sum_{\alpha=1}^n F_{\rm uz}(z_\alpha)}}, \qquad (4)$$

where the overline denotes averaging over point disorder. The averaging procedure can be easily done for a positive integer n. First we order the coordinates z_j, where the j^{th} replica unbinds from the pin according to: $0 \le z_1 \le z_2 \le \ldots \le z_n$. Then for $z \in [0, z_1)$ there are no replicas bound to the columnar pin, for $z \in [z_1, z_2)$ there is one replica on the pin until finally for $L \ge z \ge z_n$ all n replicas are bound to the pin. Using this observation and explicitly averaging over the point disorder in Eq. (4) we arrive at:

$$Z_n = n! \int\limits_{0\le z_1 \cdots \le z_n \le L} \ldots \int dz_n \ldots dz_n\, \mathrm{e}^{-\sum_{j=1}^n \epsilon z_j - \Delta/2 j^2 (z_{j+1} - z_j)} \qquad (5)$$

where we use the convention $z_{n+1} = L$. The integral above is straightforward to evaluate in the $L \to \infty$ limit:

$$\begin{aligned} Z_n &= e^{n^2\Delta/2\,L} \frac{1}{\epsilon_n^n} \prod_{j=1}^n \frac{1}{1-\kappa_n j} \\ &= e^{n^2\Delta/2\,L} \left(\frac{2}{\Delta}\right)^n \frac{\Gamma(1+1/\kappa_n - n)}{\Gamma(1+1/\kappa_n)} \equiv e^{n^2\Delta/2\,L} Q_n. \end{aligned} \qquad (6)$$

where $\epsilon_n = \epsilon + \Delta n$ and $\kappa_n = \Delta/2\epsilon_n$. The exponential prefactor is the contribution of the whole pin while the rest of the expression is the (L independent) contribution from the unzipped region. The disorder averaged free energy is given by the limit $\overline{F} = -\lim_{n\to 0}(Z_n - 1)/n$. Using Eq. (6) one obtains

$$\overline{F} = \ln(\epsilon\kappa) + \Psi(1/\kappa), \qquad (7)$$

where $\Psi(x)$ is the digamma function and $\kappa = \Delta/2\epsilon$. The unzipping transition occurs at $\epsilon = 0$ or equivalently at $\kappa \to \infty$. The expression (7) is identical to the one found in Ref. [15] using the Fokker-Planck equation approach, supporting the validity of the replica calculation.

Unbinding from a wall. Next we consider the unbinding of a directed polymer (or interface) from an attractive wall, in the presence of point disorder in the bulk of the system, in $d = 1+1$ dimensions (see Fig. 1a). The elastic free-energy of the problem is given by

$$F_{\rm ub} = \int d\tau \left[\frac{\gamma}{2}(\partial_\tau z(\tau))^2 + V(z(\tau)) + \mu(z(\tau), \tau)\right]. \qquad (8)$$

Here $z(\tau)$ denotes the distance of the polymer from the wall at position τ, γ is the line tension, $V(z)$ is a short

range attractive potential near the wall placed at $z = 0$ and $\mu(z,\tau)$ is the contribution from the point disorder. The free energy of this problem was obtained first, using a replica calculation, by Kardar [16]. For completeness, here we outline the main points of the derivation. The overall weight of paths connecting points $(0,0)$ and (z,τ), $W(z,\tau)$, can be calculated from

$$\begin{aligned} -\partial_\tau W(z,\tau) &= \left[\mu(z,\tau) + V(z) - \gamma\partial_z^2\right] W(z,\tau) \\ &= \mathcal{H}(z,\tau) W(z,\tau). \end{aligned} \quad (9)$$

After replicating the Hamiltonian n times one obtains

$$\mathcal{H}_n = -\frac{\sigma}{2}n - \sum_{\alpha=1}^{n}\left[\gamma\partial_{z_\alpha}^2 + V(z_\alpha)\right] - \sigma\sum_{\alpha<\beta}\delta(z_\alpha - z_\beta)\ , \quad (10)$$

where we have assumed a Gaussian distribution of μ with zero mean and variance σ. Averaging over disorder eliminated the z dependence of μ. The ground-state wave function ψ (as well as the energy) of the problem were obtained by Kardar using the Bethe ansatz. We skip the details as they can be found in Ref. [16]. For the permutation $\mathbf{P}$ of particles such that $0 < z_{P1} < z_{P2} < \ldots < z_{Pn}$ and below the transition $\psi \sim \exp\left(-\sum_{\alpha=1}^{n}\chi_\alpha z_{P\alpha}\right)$. Here $\chi_\alpha = \lambda + 2(\alpha-1)\chi$, $\chi = \sigma/4\gamma$ and λ depends on the strength of the attractive potential at the wall. We note that the wave function gives the probability distribution of the directed polymer at the top of the sample ($\tau = L$), and thus it is proportional to the restricted partition function $W(L,z)$. Integrating ψ over all coordinates gives the generating function of moments of z [16]:

$$N_n \equiv \int dz_1 \ldots \int dz_n\, \psi = \frac{1}{\chi^n}\frac{\Gamma(1+1/\kappa_n - n)}{\Gamma(1+1/\kappa_n)}, \quad (11)$$

where now $\kappa_n = \chi/\epsilon_n$ and $\epsilon_n = \lambda - \chi + 2\chi n$. Note that with a proper identification of ϵ_n and κ_n

$$Q_n = N_n\ . \quad (12)$$

This is the main result of our paper. In fact, one can check that not only the generating functions Q_n and N_n coincide, but also the wave function of the DPRM problem is identical (up to an unimportant constant) to the restricted partition function of the DNA unzipping problem. This equivalence implies that *below the transition* all the moments and cumulants of the unzipped length and of the distance of the polymer from the wall are equivalent. In particular, the weight of finding the DPRM a distance z from the wall for a *particular* realization of disorder is given by $Z(z)$, defined in Eq. (2). Note that the free-energies of the two models are *distinct*. Indeed Q_n contains information on the free-energy of the unzipping problem. However, for the DPRM N_n only describes the spatial distribution of z at the top of the sample. In particular, the sum over weights of a DPRM, which ends at the point z at the top of the sample, $W(z,L)$, is given by

$$W(z,L) = e^{-E_0 L}\frac{\psi(z)}{\int dz'\psi(z')} = e^{-E_0 L}\frac{Z(z)}{Z}, \quad (13)$$

where $Z(z)$ is defined in Eq. (2), E_0 is a sample dependent free-energy and Z is the normalization factor. We note that the equivalence between $\psi(z)$ and $Z(z)$ gives an example of the SMF decomposition [13] for a disordered DPRM problem corresponding to a time-dependent Hamiltonian.

It is easy to see that for both models

$$\overline{\langle z\rangle} = \partial F/\partial\epsilon = (\kappa\epsilon)^{-1}\Psi^{(1)}(1/\kappa), \quad (14)$$

where $\Psi^{(n)}(x)$ stands for the n-th derivative of the digamma function. The expression above predicts a crossover from $\overline{\langle z\rangle} \approx 1/\epsilon$ for $\kappa \ll 1$ (far from the transition) to $\overline{\langle z\rangle} \approx \kappa/\epsilon = \Delta/\epsilon^2$ for $\kappa \gg 1$ (close to the transition) as was noted previously for both unzipping [9] and unbinding [16] problems separately. Similarly

$$w = \overline{\langle z^2\rangle - \langle z\rangle^2} = \partial^2 F/\partial\epsilon^2 = -(\kappa\epsilon)^{-2}\Psi^{(2)}(1/\kappa). \quad (15)$$

Here there is a crossover from $w \approx 1/\epsilon^2$ for $\kappa \ll 1$ to $w \approx 2\kappa/\epsilon^2 = \Delta/\epsilon^3$ for $\kappa \gg 1$. As has been noted in the context of DNA unzipping $\sqrt{w}/\overline{\langle z\rangle}$ changes from being unity for $\kappa \ll 1$ to $\sim \epsilon^{1/2}$ for $\kappa \gg 1$. Thus close to the transition, thermal fluctuations become negligible.

Calculation of the second moment. With a little more work we can evaluate higher moments of the distribution. In particular, the second moment, which gives the variance. To do this we consider the generating function:

$$\mathcal{W}_n = n!\int\limits_{0\le z_n\cdots\le z_1\le\infty} dz_1\ldots dz_n\, \mathrm{e}^{-\sum\limits_{j=1}^{n}\epsilon_j z_j + \Delta/2 j^2 (z_{j-1}-z_j)}. \quad (16)$$

The second (and similarly the higher) moments can be found by differentiating $\mathcal{W}_n$ with respect to ϵ_j:

$$\overline{\langle z^2\rangle} = \lim_{n\to 0}\frac{1}{\mathcal{W}_n}\frac{1}{n}\sum_{j=1}^{n}\left.\frac{\partial^2\mathcal{W}_n}{\partial\epsilon_j^2}\right|_{\epsilon_j=\epsilon}. \quad (17)$$

Evaluating the simple integral in Eq. (16) we find that $\mathcal{W}_n = 1/\prod_{j=1}^{n}\left[\sum_{k=1}^{j}\epsilon_k - \Delta j^2/2\right]$ and correspondingly

$$\overline{\langle z^2\rangle} = \frac{1}{\epsilon^2}\lim_{n\to 0}\frac{1}{n}\sum_{j=1}^{n}\frac{2}{1-\kappa j}\sum_{k=j}^{n}\frac{1}{k(1-\kappa k)}. \quad (18)$$

This sum can be evaluated using a trick similar to the one suggested by Kardar [16]:

$$\begin{aligned} \overline{\langle z^2\rangle} &= \frac{2\kappa^2}{\epsilon^2}\iint\limits_{x>y>0} dxdy\frac{1}{\mathrm{e}^{\kappa x}-1}\frac{y\,\mathrm{e}^{-y}}{\mathrm{e}^{\kappa y}-1}\left[\mathrm{e}^{\kappa y} + \mathrm{e}^{2y}\mathrm{e}^{\kappa x - x}\right] \\ &- \frac{4}{\kappa\epsilon^2}\Psi^{(1)}(1/\kappa)\left(C + \Psi(1/\kappa)\right), \end{aligned} \quad (19)$$

where $C \approx 0.577$ is the Euler's constant. In the limit of weak disorder or high temperature $\kappa \ll 1$, not surprisingly, we get $\overline{\langle z^2\rangle} \approx 2/\epsilon^2$, which agrees with the Poissonian statistics of z with a average given by $\overline{\langle z\rangle} = 1/\epsilon$. In

the opposite limit $\kappa \gg 1$ one finds $\overline{\langle z^2\rangle} = 4\kappa^2/\epsilon^2 = 4\overline{\langle z\rangle}^2$. Thus in this limit the relative width of the distribution $\delta z/\overline{\langle z\rangle}$, where $\delta z^2 = \overline{\langle z^2\rangle} - \overline{\langle z\rangle}^2$, is larger by a factor of $\sqrt{3}$ than that in the high temperature regime. The distribution becomes superpoissonian at large κ. In fact at $\kappa \to \infty$ one can derive the full distribution function $P_{\kappa\to\infty}(z)$ using extreme value statistics [9, 17]: $\mathcal{P}_{\kappa\to\infty}(z) \approx \epsilon/\kappa\, G(z\,\epsilon/\kappa)$, with

$$G(x) = \frac{1}{\sqrt{\pi x}}\,\mathrm{e}^{-x/4} - \frac{1}{2}\mathrm{erfc}(\sqrt{x}/2), \qquad (20)$$

where $\mathrm{erfc}(x)$ is the complimentary error function. It is easy to check that this distribution indeed reproduces correct expressions for the mean and the variance. We additionally performed direct numerical simulations of the partition function (2) and got excellent agreement with predictions of Eqs. (19) and (20) [18].

The quantity $\overline{\langle z^2\rangle}$ is not always experimentally accessible. For example, in the unzipping experiments it is easier to measure thermal average, $\langle z\rangle$, in each experimental run. Then the variance of the distribution will be characterized by $\overline{\langle z\rangle^2}$. The difference between the two expectation values is given by w found in Eq. (15). Defining $\delta z_T^2 = \overline{\langle z\rangle^2} - \overline{\langle z\rangle}^2$ and using Eqs. (19) and (15) we find that $\delta z_T/\overline{\langle z\rangle} \approx \sqrt{\kappa/2}$ in the weak disorder limit ($\kappa \ll 1$) and $\delta z_T/\overline{\langle z\rangle} \approx \sqrt{3} - 1/(\sqrt{3}\kappa)$ for $\kappa \gg 1$. We plot both δz_T and δz versus the disorder parameter κ in Fig. 2. Note that importance of the order of thermal

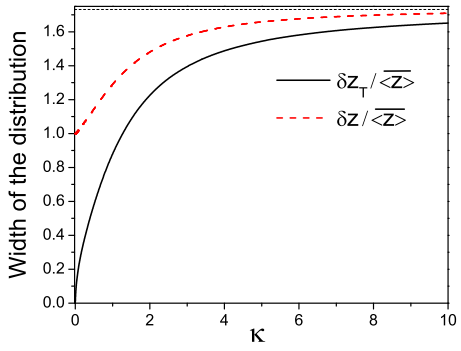

FIG. 2: Dependence of the relative width of the distribution on the disorder parameter κ. The two curves correspond to different averaging over temperature and disorder (see the text for details). The horizontal line at $\sqrt{3}$ denotes the asymptotic value of both $\delta z/\overline{\langle z\rangle}$ and $\delta z_T/\overline{\langle z\rangle}$ at $\kappa \to \infty$

and disorder averaging also appears in the calculation of higher moments of z becoming irrelevant only in the zero-temperature (strong disorder) limit ($\kappa \to \infty$).

Implications. We now turn to discuss the implications of our results for the KPZ equation and the ASEP. The height variable in the KPZ equation is well known to be related to the DPRM through the Cole-Hopf transformation $h(z,\tau) = -\ln(W(z,\tau))$. The latter together with Eq. (9) yields

$$\partial_\tau h(z,\tau) = \gamma\partial_z^2 h(z,\tau) - \gamma(\partial_z h(z,\tau))^2 + V(z) + \mu(z,\tau)\ . \qquad (21)$$

Now τ represents a time coordinate for the growing interface. The pinning potential at the origin leads to a reduced growth rate at a free boundary of the interface (for more details on the correspondence see, for example, [6]). As stated previously, the relation between the unzipping problem and the DPRM does not give the full information about $W(z,\tau)$. It only contains its spatial behavior but misses the prefactor (see Eq. (13)), which corresponds in the KPZ picture to the overall height of the interface. However, the mapping implies that up to this overall height the interface is described by Eq. (3), namely $h(z,\tau) = h_a(\tau) + F_{\rm uz}(z)$, where $h_a(\tau)$ is the mean height and $F_{\rm uz}(z)$ is a tilted random walk. The probability for an interface profile $F_{\rm uz}(z)$ is equal to the probability of drawing the random contributions $U(z)$ (see Eq. (3)). The correspondence implies, for example, that $h(z) - h(0)$ has a Gaussian distribution with a variance which increases linearly with z. The localization of the polymer near the unbinding transition corresponds to a single dominant minima in the free energy (equivalent to a minimum in the interface), the average distance of these minima from the interface behaves as $1/\epsilon^2$ (see the discussion after Eq. (14)).

Next, we turn to implications of our results for the ASEP. We consider a semi-infinite system where particles hop into a one dimensional lattice at the left end with a rate α and hop in the bulk of the system to the nearest neighbor on the right with a rate 1. In the continuum limit the behavior of the system is captured by the equation [5]

$$\partial_\tau \rho(z) = -\frac{1}{2}\partial_z^2\rho(z) + 2\rho(z)\partial_z\rho(z) - \partial_z\rho(z) + U(x) + \eta(z,\tau)\ . \qquad (22)$$

where $U(x)$ represents injection of particles into the system and $\eta(z,\tau) = \partial_z\mu(z,\tau)$ (with $\mu(z,\tau)$ as before drawn from a Gaussian distribution) is a conserving noise. The equation can be obtained from Eq. (21) by setting $\gamma = 1/2$ and defining a variable $m(z,\tau) = (z - h(z,\tau))/2$ (note that $\partial_z h(z,\tau)$ satisfies the noisy Burgers equation). It is straightforward to verify that $\rho(z,\tau) = \partial_z m(z,\tau)$ indeed satisfies Eq. (22). Using the same reasoning as in the KPZ equation we find that in the steady state the density profile is described by $\rho(z) = (1 - \epsilon - U(z))/2$. This result suggests that in a discrete realization of the model a particle appears at a given site with a constant probability and there are no correlations between different sites. Our results hold, in ceratin limits, even when another boundary is included in the system. For example when at the other end the particles are ejected at a high rate. Indeed it is known that for the ASEP with open boundaries the density is flat near the end where particles are injected into the system [6, 7]. However, we

emphasize the *lack of correlations* near the left boundary arbitrarily close to a continuous transition. Similarly, for the interface growth with two boundaries our results apply if the growth rate is sufficiently slow only near one of the walls. We have performed numerical simulation which verified these statements. These results will be presented elsewhere [18].

In conclusion, we demonstrated that there is exact mapping between the partition function of the DNA unzipping transition and the spatial distribution of a DPRM unbinding from a wall. This mapping allowed us to apply some known and newly derived results of the simpler unzipping problem to the DPRM problem. We also showed how this mapping can be used to derive results for the KPZ equation near a boundary and about asymmetric exclusion process with open boundaries.

We would like to acknowledge D. R. Nelson for useful discussions and collaboration on a related work. We are also grateful for illuminating discussions to C. Castelnovo, C. Chamon, and M. R. Evans. YK would like to thank the Newton Institute in Cambridge, UK where part of the work was carried out. Work by Y. K. was supported by the United States-Israel Binational Science Foundation (BSF) through Grant. No. 2004072.

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[19] We note that there is a slight correction to this expression, because the line, once it leaves the potential, is not allowed to return. However, this correction will be negligible near the unzipping transition, where z is large.